

## Chemistry 430 — Simulation in Chemistry & Biochemistry

Laboratory Report Format:

In order to complete this project, you should write a "lab report" with the sections outlined below. These should be turned in to Jay Ponder (email or in person), preferably within about two weeks following the date of the lab period.

- (1) Introduction -- brief summary and reason for doing the project
- (2) Procedure -- what steps did you actually perform, and in what order
- (3) Methods -- kinds of calculations, programs used, level of theory, any assumptions or approximations such as quantities varied, restraints and constraints, special program options, *etc.*
- (4) Results -- data obtained, usually presented as both tables and plots
- (5) Analysis -- explain your results; why did things turn out as they did, what can you find in texts or published papers to support your interpretation of the data (*i.e.*, for this specific system or for analogous systems)
- (6) Conclusions -- what lessons were learned from this project, what kinds additional calculations could be done to further explore the topic
- (7) Questions -- answer specific questions provided as part of the project